

Isotropic matrix elements of the Boltzmann equation collision integral.

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We propose an algorithm for calculating matrix elements of the non-linear Boltzmann equation collision integral in isotropic case. These matrix elements are used as starting ones in the recurrence procedure for calculating the matrix elements of the collision integral, which is non-isotropic with respect to velocities, as described in our previous paper. In addition, isotropic matrix elements are of independent interest for the calculation of isotropic relaxation in a number of problems of physical-chemical kinetics. It is shown that the coefficients of the isotropic matrix elements expansion in terms of Ω -integrals are connected by recurrence relations that allow us to calculate them sequentially.

1 Introduction

The progress of modern technology both due to miniaturization of devices and more intense operating modes requires to treat kinetic problems by consideration of the distribution function (DF). Knowledge of the distribution function at high values of the velocities turns out to be decisive for the calculation of physical-chemical processes in gas and plasma. Finally, the natural evolution of the kinetic theory itself leads to the necessity of developing methods for calculating the distribution function that is far from equilibrium. One of the methods for solving the Boltzmann equation for a system that deviates strongly from equilibrium is the method of polynomial expansions, in particular, the moment method in which the distribution function is expanded in terms of Barnett functions $H_{r,l,m} = S_{l+1/2}^r(x)Y_{l,m}(\theta, \phi)$, where $S_{l+1/2}^r(x)$ are Sonine polynomials.

The main drawback of this method was the lack of sufficient number of computed collision integral matrix elements (ME). As a rule, non-isotropic ME with small indices l were calculated in the kinetic theory of gases [1, 2]. This is due to their great importance for the calculation of the transport coefficients in the case of small deviations from equilibrium. In highly nonequilibrium processes, accurate calculation of the distribution function requires matrix elements with large indices. The analytical formula for ME (see, for example, [3]) are extremely cumbersome. In [4, 5], a much simpler method to determine ME sequentially using recurrence procedures has been proposed.

The present paper is closely related to our previous work [6], which describes the recurrence procedure for constructing any non-isotropic (corresponding to a velocity-non-isotropic distribution function) matrix elements. The isotropic ME are used in the procedure as starting ones. It is important to note that information about interaction cross sections is used only at the stage of isotropic ME calculation. It will be shown in the paper that any isotropic MEs, both linear and non-linear, can be represented as a linear combination of Ω -integrals whose coefficients are related by algebraic recurrence relations.

It should be noted that the calculation of isotropic ME is important not only to complete our recurrent procedure. Recently, an article by Shizgal and Drydy [7] appeared, in which the expansion coefficients of linear isotropic MEs in terms of Ω integrals are calculated. This article describes a number of applied problems where linear isotropic ME are necessary. This is important, for example, in the calculation of a distribution function of small quantity of the atoms (or ions) in the equilibrium gas of atoms of another kind.

In [7], the importance of the isotropic relaxation, i.e. stage at which the DF relaxes, remaining isotropic is emphasized. The rates of physical-chemical processes physical-chemical transformations at this stage are determined by the behaviour of the DF at high velocities.

Thus, the expansion of isotropic matrix elements in Ω -integrals is important both to obtain starting ME for the recurrence procedure and, as itself, to solve relaxation

problems, in particular, for physical-chemical kinetics.

2 Statement of the problem

Non-linear collision integrals for each pair of gas mixture components with masses m_a and m_b and densities n_a and n_b for isotropic distribution function ($f_a(\mathbf{v}) = f_a(v)$) have the form:

$$\hat{I}(f_a, f_b) = n_a n_b \int (f_a(v_1) f_b(v_2) - f_a(v) f_b(v')) g \sigma_{ab}(g, \theta) d\mathbf{v}' d\mathbf{k}. \quad (1)$$

The particle velocities before and after the collision are related by

$$\begin{aligned} \mathbf{v}_1 &= \mathbf{v}_0 - \mu_b \mathbf{k} g, & \mathbf{v}_2 &= \mathbf{v}_0 + \mu_a \mathbf{k} g, & \mathbf{v}_0 &= (\mu_a \mathbf{v} + \mu_b \mathbf{v}'), \\ \mu_a &= m_a / (m_a + m_b), & \mu_b &= m_b / (m_a + m_b), \\ \mathbf{g} &= \mathbf{v}_1 - \mathbf{v}_2, & \mathbf{g}' &= \mathbf{v} - \mathbf{v}', & g &= g', \end{aligned} \quad (2)$$

where \mathbf{k} is unit vector, directed along \mathbf{g} . The scattering angle θ is determined by the relation $\cos \theta = \mathbf{k} \cdot \mathbf{g}' / g$, and $\sigma_{ab}(g, \theta)$ is the differential scattering cross section.

When applying the moment method to isotropic problems, the distribution function of the a -th component of the mixture $f_a(v)$ is expanded in Sonin polynomials $S_{1/2}^r(x)$ with the Maxwellian weight M_a

$$f_a(v, t) = M_a \sum_{r=0}^{\infty} C_r^a(t) S_{1/2}^r \left(\frac{m_a v^2}{2kT} \right), \quad M_a = \left(\frac{m_a}{2kT\pi} \right)^{3/2} \exp \left(\frac{-m_a v^2}{2kT} \right). \quad (3)$$

Here k is the Boltzmann constant, and T is the temperature of the weighted Maxwellian. The isotropic matrix elements $(K_{a,b}^a)_{r_1, r_2}^r$ are defined in terms of the collision integrals $\hat{I}(f_a, f_b)$ as follows:

$$(K_{a,b}^a)_{r_1, r_2}^r = \frac{4\pi}{\nu_r} \left(\int_0^{\infty} S_{1/2}^r(c_a^2) \hat{I}_{a,b}(M_a S_{1/2}^{r_1}(c_a^2), M_b S_{1/2}^{r_2}(c_b^2)) v^2 dv \right), \quad (4)$$

$$c_a = \left(\frac{m_a}{2kT}\right)^{1/2} v, \quad c_b = \left(\frac{m_b}{2kT}\right)^{1/2} v, \quad \nu_r = \frac{(2r+1)!!}{(2r)!!}. \quad (5)$$

In a more general, non-isotropic case, ME are defined by a formula similar to (4), however, Barnett's functions $H_{r,l,m} = S_{l+1/2}^r(x)Y_{l,m}(\theta, \phi)$ are used as the basis functions instead of Sonine polynomials, where $Y_{l,m}(\theta, \phi)$ are spherical harmonics.

As it was shown in [8, 4], isotropic ME ($K_{a,b}^a$) with different indices are related by

$$\begin{aligned} T \frac{d(K_{a,b}^a)_{r_1,r_2}^r(T)}{dT} - (r_1 + r_2 - r)(K_{a,b}^a)_{r_1,r_2}^r(T) = \\ = r(K_{a,b}^a)_{r_1,r_2}^{r-1}(T) - (r_1 + 1)(K_{a,b}^a)_{r_1+1,r_2}^r(T) - (r_2 + 1)(K_{a,b}^a)_{r_1,r_2+1}^r(T). \end{aligned} \quad (6)$$

In the case of a power-law dependence of the potential φ on the distance r ($\varphi \sim 1/r^\kappa$) the cross section is represented in the form

$$\sigma_{ab}(g, \theta) = g^{\gamma-1} F_\gamma^{ab}(z). \quad (7)$$

Here $z = \sin^2(\theta/2)$, $\gamma = (\kappa - 4)/\kappa$, $F_\gamma^{ab}(\theta)$ is the angular part of cross section, θ is the scattering angle.

In the case of scattering cross section (7) the ME is proportional to T^μ , where $\mu = \gamma/2$ (see, e.g. [9]).

Relations (6) become algebraic recurrence relations:

$$\begin{aligned} (\mu - r_1 - r_2 + r)(K_{a,b}^a)_{r_1,r_2}^r(T) = \\ = r(K_{a,b}^a)_{r_1,r_2}^{r-1}(T) - (r_1 + 1)(K_{a,b}^a)_{r_1+1,r_2}^r(T) - (r_2 + 1)(K_{a,b}^a)_{r_1,r_2+1}^r(T). \end{aligned} \quad (8)$$

The relations (8) allow us to establish the recurrence procedure for sequential determination of ME and linear ME $K_{r_1,0}^r$ (first type) or K_{0,r_2}^r (second type) are the starting ones. The simple analytical formulas for these starting ME were obtained [8, 4] in the case of a monoatomic gas. On the basis of recurrence relations (8) we have created a program for calculating ME with large indices (with indices of the order of hundreds or more), for which it turned out necessary to develop special procedures to perform calculations with large amount of significant digits. This

made it possible to solve the non-linear Boltzmann equation in the isotropic case and calculate the distribution function in the range of up to 8-10 thermal velocities. For Maxwellian molecules, calculations were made up to 12 thermal velocities. The comparison with the analytical solution of the BKW [10] was made and the complete coincidence was observed. In this case, the ratio of the distribution function to the equilibrium Maxwellian was considered.

In the case of arbitrary interaction laws, the calculation of linear nonisotropic MEs for small values of the index l ($l = 1, 2$), corresponding to the expansion of the DF in spherical harmonics, is analytically carried out in [1, 2]. As a result, such MEs are represented as a linear combination of double integrals (Ω -integrals) containing the cross section of the interaction $\sigma_{ab}(g, \theta)$.

Following [2], we write Ω -integrals in the form

$$\Omega_{ab}^{(n,m)} = \left(\frac{kT}{2\pi m_{ab}} \right)^{1/2} \int_0^\infty e^{-\bar{g}^2} \bar{g}^{2m+3} Q_{ab}^{(n)} d\bar{g}, \quad (9)$$

where $m_{ab} = (m_a m_b)/(m_a + m_b)$ is the reduced mass of a pair of molecules a and b , and the dimensionless integration variable $\bar{g} = g\sqrt{m_{ab}/2kT}$. The value of $Q_{ab}^{(n)}$ in (9) is determined by the expression

$$Q_{ab}^{(n)} = 2\pi \int_0^\pi (1 - \cos^n \theta) \sigma_{ab}(g, \theta) \sin \theta d\theta. \quad (10)$$

Analytic representations of isotropic linear MEs of both first and second types in the form of finite sums of Ω -integrals are obtained in [11] by analogy with the method of calculating integral brackets [1, 2], which is well known from the kinetic theory. In this case, just as in [1, 2], the generating function for Sonine polynomials is used, the same integration variables are chosen, and the orders of numerous summations are changed in the same way. In the isotropic case, the calculations turned out to be much simpler. It is especially simple to express linear isotropic ME of the second type K_{0,r_2}^r through Ω -integrals. Therefore we choose the expansion coefficients of these ME as the starting ones to calculate all isotropic ME by recurrence procedure.

In this case, instead of the functions $Q_{ab}^{(n)}$, it is convenient to use

$$Q_{*ab}^{(n)} = 2\pi(1 - \delta_{n,0}) \int_0^\pi (1 - \cos \theta)^n \sigma_{ab}(g, \theta) \sin \theta \, d\theta. \quad (11)$$

By analogy with Ω -integrals, we define Ω_* - integrals

$$\Omega_{*ab}^{(n,m)} = \left(\frac{kT}{2\pi m_{ab}} \right)^{1/2} \int_0^\infty e^{-\bar{g}^2} \bar{g}^{2m+3} Q_{*ab}^{(n)} \, d\bar{g}. \quad (12)$$

Ω_* - integrals can be easily expressed in terms of Ω -integrals, and conversely:

$$\Omega_{*ab}^{(n,m)} = \sum_{l=0}^n \binom{n}{l} (-1)^{l+1} \Omega_{ab}^{(l,m)}, \quad \Omega_{ab}^{(n,m)} = \sum_{l=1}^n \binom{n}{l} (-1)^{l+1} \Omega_{*ab}^{(l,m)}. \quad (13)$$

We give here the representations of linear isotropic ME of the first and second types obtained in [11] via Ω_* - integrals. For ME of the first type, we have

$$K_{p,0}^q = (-1)^{p+q} \sum_{n=1}^{\min(p,q)} \sum_{m=n}^{p+q-n} A_{p,q;n,m}^{*(1)} \Omega_{*ab}^{(n,m)}, \quad (14)$$

$$A_{p,q;n,m}^{*(1)} = 8\nu_q^{-1} \mu_a^n \mu_b^m \sum_{j=j_0}^{m-n} \frac{2^{m-j}}{n! j! (m-j-n)!} \sum_{i=i_0}^{s-2m} G_{pqjim}, \quad (15)$$

$$G_{pqjim} = \frac{(-1)^{i+n} \mu_b^i (1 - \mu_a/\mu_b)^{s-i-2m}}{(i+m-p)!(i+m-q)!(s-i-2m)!} \times \\ \times \frac{\Gamma(i+m+3/2)(2(i+m)+j-s)!}{\Gamma(m+3/2)(2(i+m)-s)!}, \quad s = j+p+q.$$

Here

$$j_0 = \max(0, m-p, m-q, 2m-p-q), \quad i_0 = \max(0, p-m, q-m, (j+p+q-2m)/2).$$

Matrix elements of the second type are expressed in terms of Ω_* - integrals as follows

$$(K_{a,b}^a)_{0,p}^q = -8\nu_q^{-1} \mu_b^p \mu_a^q \sum_{n=1}^{\min(p,q)} \sum_{m=n}^{p+q-n} A_{p,q;n,m}^* \Omega_{*ab}^{(n,m)}, \quad (16)$$

where

$$A_{p,q;n,m}^{*(2)} = \frac{2^n \Gamma(p+q-n+3/2)}{n!(p-n)!(q-n)!} \binom{p+q-2n}{m-n} \frac{(-1)^{m+n}}{\Gamma(m+3/2)} \quad (17)$$

From these formulas it is clear that the representation of ME of the second type in terms of Ω_* - integrals is much simpler. Therefore, it is natural to start the recurrent procedure with ME of the second type.

3 Derivation of non-linear matrix elements

Let us show that starting with linear ME of the second type (16) and using the relations (6) one can construct all isotropic MEs, both non-linear and linear of the first type. Despite the fact that (6) includes the ME derivative with respect to temperature, the relationships between the coefficients of the ME expansion in Ω -integrals, as will be shown below, turn out to be algebraic.

Taking into account (13), it is easy to see that Ω_* - integrals are related to each other in the same way as Ω -integrals ([2])

$$T \frac{\partial \Omega_{*ab}^{(n,m)}}{\partial T} + (m+3/2) \Omega_{*ab}^{(n,m)} = \Omega_{*ab}^{(n,m+1)}. \quad (18)$$

We write the recurrence relation (6) in the form

$$\begin{aligned} (r_1+1)(K_{a,b}^a)_{r_1+1,r_2}^r &= -(r_2+1)(K_{a,b}^a)_{r_1,r_2+1}^r - T \frac{d(K_{a,b}^a)_{r_1,r_2}^r}{dT} \\ &+ (r_1+r_2-r)(K_{a,b}^a)_{r_1,r_2}^r + r(K_{a,b}^a)_{r_1,r_2}^{r-1}. \end{aligned} \quad (19)$$

In what follows, it is convenient to use not r_2 , but $N = r_1 + r_2$ as the second lower index in the matrix element $(K_{a,b}^a)_{r_1,r_2}^r$. We denote the corresponding ME by $K_{r_1,N}^{'r}$, i.e.

$$K_{r_1,N}^{'r} = (K_{a,b}^a)_{r_1,N-r_1}^r. \quad (20)$$

In this notation, after the replacement of N by $N - 1$ (19) takes the form

$$\begin{aligned} (r_1 + 1)K'_{r_1+1,N} = & -(N - r_1)K'_{r_1,N} - T \frac{d}{dT} K'_{r_1,N-1} + \\ & + (N - 1 - r)K'_{r_1,N-1} + rK'_{r_1,N-1}^{r-1}. \end{aligned} \quad (21)$$

In accordance with (16) and (20) for $r_1 = 0$ we have

$$K'_{0,N} = \sum_{n=1}^{\min(N,r)} \sum_{m=n}^{N+r-n} \beta_{0,N}^r(n, m) \Omega_{*ab}^{(n,m)}, \quad (22)$$

where

$$\beta_{0,N}^r(n, m) = 8\nu_r^{-1} \mu_b^N \mu_a^r A_{N,r;n,m}^*. \quad (23)$$

Thus $K'_{0,N}$ is a linear combination of Ω_* - integrals, where summation indices n and m vary in the range

$$1 \leq n \leq \min(N, r), \quad n \leq m \leq N + r - n. \quad (24)$$

Let us consider the recurrence relation (21) for $r_1 = 0$. First, using (18), we rewrite the term containing the derivative:

$$\begin{aligned} T \frac{d}{dT} K'_{0,N-1} = & \sum_{n=1}^{\min(N-1,r)} \sum_{m=n+1}^{N+r-n} \beta_{0,N-1}^r(n, m) \Omega_{*ab}^{(n,m+1)} - \\ & - \sum_{n=1}^{\min(N-1,r)} \sum_{m=n}^{N-1+r-n} (m + 3/2) \beta_{0,N-1}^r(n, m) \Omega_{*ab}^{(n,m)}. \end{aligned} \quad (25)$$

Passing in the first of the double sums in (25) from the summation variable m to $m - 1$ and substituting the result in (21), we get

$$\begin{aligned} K'_{1,N} = & -NK'_{0,N} + (N - 1 - r)K'_{0,N-1} + rK'_{0,N-1}^{r-1} - \\ & - \sum_{n=1}^{\min(N-1,r)} \sum_{m=n+1}^{N+r-n} \beta_{0,N-1}^r(n, m - 1) \Omega_{*ab}^{(n,m)} + \end{aligned}$$

$$+ \sum_{n=1}^{\min(N-1,r)} \sum_{m=n}^{N-1+r-n} (m+3/2) \beta_{0,N-1}^r(n,m) \Omega_{*ab}^{(n,m)}. \quad (26)$$

That is, the limits of summation over n and m do not extend when $K'_{0,N}$ is differentiated with respect to temperature. Substituting the expression for $K'_{0,N}$ (22) in (26), we obtain the expansion of $K'_{1,N}$ in the Ω_* integrals that has the same structure as (22). Note that the summation limits (24) does not change in this case. Consistently increasing r_1 , one can show in the same way that in the general case the limits of summation in expression for $K'_{r_1+1,N}$ do not depend on r_1 , and arbitrary matrix element is represented as a linear combination

$$K'_{r_1,N} = \sum_{n=1}^{\min(N,r)} \sum_{m=n}^{N+r-n} \beta_{r_1,N}^r(n,m) \Omega_{*ab}^{(n,m)}, \quad (27)$$

It is clear that the same formula with other coefficients is also valid for the expansion in Ω -integrals.

Let us extend the matrix $\beta_{r_1,N}^r(n,m)$ setting the elements with $n > \min(N,r)$ and $m > N+r-n$ equal to zero. Then we can write

$$K'_{r_1,N} = \sum_{n=1}^{\infty} \sum_{m=n}^{\infty} \beta_{r_1,N}^r(n,m) \Omega_{*ab}^{(n,m)}.$$

Substituting the last equality in (21) and equating the coefficients for the same Ω_* integrals, we obtain the following recurrence relation, where θ -functions explicitly identify ranges of indices where $\beta_{R_1,N}^r(n,m)$ are non-zero

$$\begin{aligned} \beta_{r_1+1,N}^r(n,m) = & \frac{1}{r_1+1} \left[-(N-r_1) \times \right. \\ & \times \Theta(\min(N,r) - n) \Theta(N+r-n-m) \beta_{r_1,N}^r(n,m) + (m+N-1-r+3/2) \times \\ & \times \Theta(\min(N-1,r) - n) \Theta(N-1+r-n-m) \beta_{r_1,N-1}^r(n,m) + \\ & + r \Theta(\min(N-1,r-1) - n) \Theta(N+r-2-n-m) \beta_{r_1,N-1}^{r-1}(n,m) - \\ & \left. - \Theta(\min(N-1,r) - n) \Theta(N+r-n-m) (1 - \delta_{m,n}) \beta_{r_1,N-1}^r(n,m-1) \right]. \quad (28) \end{aligned}$$

The same recurrence formula is valid for the expansion in Ω -integrals. The only difference is in the initial expansion coefficients $\beta_{0,N}^r(n, m)$. We especially note that for any fixed mass ratio the recurrence formula (28) for the matrix β is universal and does not depend on the interaction cross section.

We wrote a program for calculating the matrix β by the formula (28). The obtained coefficients of the expansion of the linear isotropic ME of the first type $(K_{a,b}^a)_{0,p}^q$ in Ω -integrals, coincide with ones that analytically found in [13] for several first indices. We emphasize that these MEs are calculated at the final step of the recurrence procedure after the determination of all non-linear ME.

Thus, it is shown that the connections between MEs can be used as recurrence relations in the calculation of non-linear ME for arbitrary interaction laws.

Note that the calculation of the expansion coefficients $\beta_{r_1,N}^r(n, m)$ should be carried out with high accuracy. To implement the calculation, taking into account a large number of significant digits, we used the package MPFUN2015 [14]. We compared isotropic non-linear ME K_{r_1,r_2}^r (15 significant digits) with indices in the range $[0, 32]$ calculated using the formulas (27), (28) and determined by the recurrence relations (8) for the case of hard spheres. A complete coincidence of the results has been observed.

4 Power interaction law

Let us derive the expression for $\Omega_{*ab}^{(n,m)}$ in the case of power interaction law. Substituting the cross section (7) into the expression for $Q_{*ab}^{(n)}$ (11), after integrating over \bar{g} , we get

$$\Omega_{*ab}^{(n,m)} = 2^{\mu-2} \pi^{-1/2} \left(\frac{kT}{m_{ab}} \right)^{\mu} 2^n J_n(\mu) \Gamma(m + 3/2 + \mu), \quad (29)$$

Here $J_n(\mu)$, unlike the case of arbitrary potentials, is determined by the angular part of the cross section only:

$$J_n(\mu) = 4\pi \int_0^1 F_{\gamma}^{ab}(z) z^n dz. \quad (30)$$

Let us show that in this case the expression for linear isotropic ME of the second kind, which are the starting ones in the recurrence procedure based on (8), are much simpler than in the general case. To do this, we substitute the Ω_{*ab} (29) into the expansion (16) - (17):

$$K_{0,p}^q = -\frac{2^{\mu+1}}{\pi^{1/2}\nu_q} \left(\frac{kT}{m_{ab}}\right)^\mu \mu_b^p \mu_a^q \sum_{n=1}^{\min(p,q)} J_n(\mu) \frac{2^{2n} \Gamma(p+q-n+3/2)}{n!(p-n)!(q-n)!} \times \\ \times \sum_{s=0}^{p+q-2n} \binom{p+q-2n}{s} (-1)^s \frac{\Gamma(n+s+3/2+\mu)}{\Gamma(n+s+3/2)}. \quad (31)$$

Using the integral representation of the B -function [15], it can be shown that

$$\sum_{k=0}^t \binom{t}{k} (-1)^k \frac{\Gamma(a+k)}{\Gamma(b+k)} = \frac{\Gamma(a)\Gamma(t+b-a)}{\Gamma(b-a)\Gamma(t-b)} \quad a > 0, b > 0. \quad (32)$$

Replacing the last sum in (31) by the expression (32) for $t = p+q-2n$, $a = n+3/2+\mu$, and $b = n+3/2$, we obtain the linear isotropic ME of the second type in the form of a single sum

$$K_{0,p}^q = \left(\frac{2kT}{m_{ab}}\right)^\mu \mu_b^p \mu_a^q \frac{q!}{\Gamma(q+3/2)} \sum_{n=1}^{\min(p,q)} J_n \frac{2^{2n} \Gamma(n+3/2+\mu) \Gamma(p+q-2n-\mu)}{n!(p-n)!(q-n)! \Gamma(-\mu)}. \quad (33)$$

Thus, in the case of power interaction law, a simple formula is obtained for linear isotropic ME of the second type with an arbitrary mass ratio. This formula for a monoatomic gas ($\mu_a = \mu_b = 1/2$, $m_{ab} = m/2$) coincide with the expression obtained earlier by other method in [8, 4].

Let us express J_n in terms of the parameters of the power potential. It follows from (10) that for power potentials

$$Q_{*ab}^{(n)} = g^{2\mu-1} 2^n J_n(\mu). \quad (34)$$

Consider the potential

$$\varphi = \left(\frac{\epsilon}{r}\right)^\nu, \quad \nu = \frac{4}{1-2\mu}. \quad (35)$$

It is known (see, for example, [2]), that in the case of the potential (35) $Q_{ab}^{(n)}$ (10) can be represented in the form

$$Q_{ab}^{(n)} = 2\pi\epsilon^2 \left(\frac{m_{ab}g^2}{2\nu}\right)^{-2/\nu} A_n(\nu), \quad (36)$$

where

$$A_n(\nu) = \int_0^\infty (1 - \cos^n(\theta(s, \nu))) s ds. \quad (37)$$

The method of constructing the angle $\theta(s, \nu)$ can be found, for example, in [2]. The values of $A_n(\nu)$ for $n = 1, 2$ for a set of integer values ν in the range $4 \leq \nu \leq \infty$ are also given there.

An analogous formula is valid for $Q_{*ab}^{(n)}$

$$Q_{*ab}^{(n)} = 2\pi\epsilon^2 \left(\frac{m_{ab}g^2}{2\nu}\right)^{-2/\nu} \tilde{A}_n(\nu), \quad (38)$$

where

$$\tilde{A}_n(\nu) = \int_0^\infty (1 - \cos(\theta(s, \nu)))^n s ds. \quad (39)$$

Substituting (38) to (34) we get

$$J_n(\mu) = \pi\epsilon^2 \left(\frac{m_{ab}}{2\nu}\right)^{-2/\nu} \tilde{A}_n(\nu). \quad (40)$$

Thus, the value $J_n(\mu)$ in (33) is completely defined.

5 Conclusion

When calculating highly non-equilibrium distribution functions by the moment method, it is necessary to take into account a large number of terms in the expansion of the distribution function, hence, matrix elements with large indices are necessary. In our papers [8, 4] it is shown that MEs with neighbouring indices are connected by the relations that follow from the invariance of the collision integral with respect to the choice of the Maxwellian weight parameters in the Barnett

expansion, namely, temperature and mean velocity.

In the case of power interaction law, all the relations connecting ME are algebraic. This allowed us to construct a recurrence procedure for sequential determination of the ME [8, 4]. The obtained matrix elements were used to calculate the distribution function in the case of strong deviation from equilibrium, in particular, in strong constant and variable external fields [16].

For arbitrary laws of interaction, the relations connecting non-isotropic MEs (they follow from invariance with respect to the choice of the mean velocity of the weight Maxwellian) are also algebraic. On their basis, a recurrence procedure was constructed in [6], which allows finding all non-isotropic MEs if isotropic MEs are known. Thus, the construction of isotropic ME acquires special significance.

For arbitrary (not power-law) laws of interaction, the relations connecting isotropic ME include a derivative with respect to temperature. The use of Ω -integrals well-known in the kinetic theory allows to reduce the relations to algebraic ones. Taking into account that the derivative of the Ω -integral with respect to temperature is expressed in terms of a linear combination of Ω -integrals, it is possible to obtain algebraic relations for the coefficients of the ME expansion in Ω -integrals.

It turned out that it is more convenient to consider the coefficients of the expansion in Ω_* - integrals (12), which are easily expressed in terms of Ω -integrals. These coefficients are sequentially determined using the recurrence procedure described in this paper, and it is advisable to use the expansion coefficients of linear isotropic ME of the second type K_{0,r_2}^r , which have the simplest form (17). It should be noted that the relations connecting the expansion coefficients are common for Ω_* and Ω -integrals, they also do not depend on the masses of the colliding particles. The mass ratio enters only in the initial expansion coefficients (17).

We have implemented a procedure that allows us to compute sequentially all isotropic MEs using a set of known (tabulated) Ω -integrals. It requires computations with increased accuracy, for which the MPFUN2015 [14] package was used. The program was tested by the ME calculation for the hard sphere model.

For power interaction laws, the expansion of linear isotropic ME of the second

type in Ω_* integrals is reduced to a single sum. This representation made it possible to generalize the formula obtained in [8, 4] to the case of an arbitrary mass ratio.

For arbitrary interaction laws, isotropic non-linear ME can be calculated by the formula (27), in which the coefficients $\beta_{r_1+1,N}^r(n, m)$ are determined by the use of a recurrence procedure. In turn, as mentioned above, they are the starting values for calculating non-isotropic non-linear ME.

Thus, the use of the both recurrence procedures described in this article and in our previous article [6] makes it possible to find all the ME of the non-linear collision integral for arbitrary laws of interaction and arbitrary masses of the colliding particles. Tabulated matrix elements can then be used to solve various problems. This greatly expands the application of the moment method, which can now be used to calculate highly non-equilibrium distribution functions in real physical situations.

References

- [1] *Chapman S, Cowling TG.* The mathematical theory of non-uniform gases. Cambridge: Cambridge University Press 1939.
- [2] *J.H.Fertziger, H.G.Kaper.* Mathematical theory of Transport Processes in Gases. Amsterdam: North-Holland Publishing Company 1972.
- [3] *Viehland L.A., Maeson E.A.* // Ann. Phys. 1978. Vol. 110. P. 287?-328.
- [4] *Ender A.Ya, Ender I.A.* Collision integral of the Boltzmann equation and the moment method. St.-Petersburg, 2003. (in Russian)
- [5] *Ender A.Ya., Ender I.A.* // Transport Theory and Stat. Phys. 2007. Vol. 56. P. 563–588.
- [6] *Ender I.A., Bakaleinikov L.A., Flegontova E.Yu., Gerasimenko A.B.* // Technical Physics. 2017 (in print)
- [7] *Shizgal B. D., Dridi R.* // Computer Physics Communications. 2010. Vol. 181. P. 1633–1640
- [8] *Ender A.Ya., Ender I.A.* // Phys. Fluids. 1999. Vol. 11. P. 2720–2730.
- [9] *Ender A.Ya., Ender I.A.* // Technical Physics. 1994. V. 64. I. 10. pp. 38–53
- [10] *Bobylev A. V.* // Proc. USSR Acad. Sci. 225, 1041 (1975).
- [11] *Ender A.Ya., Ender I.A., Lutenko M.B.* Polinomial expansion for isotropic Boltzmann equation and invariance of collision integral from basis functions set. Preprint Ioffe Institute No.1716. St-Petersburg., 1998. 62 p.
- [12] *Ender A.Ya., Ender I.A.* // Phys. Fluids. 1999; 11: 2720–2730.
- [13] *Mason E.A., McDaniel E.W.* Transport Properties of Ions in Gases. Wiley, New York, 1988.

- [14] David H. Bailey MPFUN2015: A thread-safe arbitrary precision package.
<http://www.davidhbailey.com/dhbsoftware/>
- [15] Gradshtein I. S., Ryzhik I. M., Table of Integrals, Series, and Products (Nauka, Moscow, 1971; Academic, New York, 1980).
- [16] Ender A.Y., Ender I.A. and Gerasimenko A.B. // The Open Plasma Phys. J. 2009. Vol. 2. P. 24–62.